LA-UR- 04-3890

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Submitted to: ANS Winter Meeting, Washington, D.C., November 14-18, 2004

Los Alamos
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An Improved Method for Treating Monte Carlo-Diffusion Interfaces

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INTRODUCTION

Discrete Diffusion Monte Carlo (DDMC) has been suggested as a technique for increasing the efficiency of Monte Carlo simulations in diffusive media [1–3]. In this technique, Monte Carlo particles travel discrete steps between spatial cells according to a discretized diffusion equation. An important part of the DDMC method is the treatment of the interface between a transport region, where standard Monte Carlo is used, and a diffusive region, where DDMC is employed. Previously developed DDMC methods [1,2] use the Marshak boundary condition [4] at transport diffusion-interfaces, and thus produce incorrect results if the Monte Carlo-calculated angular flux incident on the interface surface is anisotropic.

In this summary we present a new interface method based on the asymptotic diffusion-limit boundary condition [5], which is able to produce accurate solutions if the incident angular flux is anisotropic. We show that this new interface technique has a simple Monte Carlo interpretation, and can be used in conjunction with the existing DDMC method. With a set of numerical simulations, we demonstrate that this asymptotic interface method is much more accurate than the previously developed Marshak interface method.

THE DDMC METHOD AND INTERFACE TECHNIQUES

We begin by considering a steady-state planar-geometry transport problem, in which a region $X_L < x < X_R$ has been designated for simulation by DDMC. In this region, the scalar flux ϕ can be approximated by the solution of the following diffusion equation,

$$-\frac{d}{dx}\frac{1}{3\Sigma_t}\frac{d\phi}{dx} + \Sigma_a\phi = Q \quad . \tag{1}$$

where Σ_t is the total cross-section, Σ_a is the absorption cross-section, and Q is the source.

We now develop a cell-centered finite-difference discretization for Eq. (1), which will govern our DDMC method. Dividing the DDMC region into a spatial grid $X_L = x_{1/2} < x_{3/2} < \cdots < x_{I+1/2} = X_R$ consisting of I cells, the standard cell-centered discretization of Eq. (1) in interior cells $2 \le i \le I-1$ is [6]:

$$\left(\frac{A_{i+1/2}}{\Delta x_i} + \frac{A_{i-1/2}}{\Delta x_i} + \Sigma_{a,i}\right)\phi_i = Q_i + \frac{A_{i+1/2}}{\Delta x_i}\phi_{i+1} + \frac{A_{i-1/2}}{\Delta x_i}\phi_{i-1} \quad , \tag{2}$$

In Eq. (2), we have used appropriate cell-averaged values of the cross-sections, source, and scalar flux, $\Delta x_i = x_{i+1/2} - x_{i-1/2}$ is the width of cell i, and $A_{i+1/2}$ is given by

$$A_{i+1/2} = \frac{2}{3}\frac{1}{\Sigma_{t,i}\Delta x_i + \Sigma_{t,i+1}\Delta x_{i+1}} \quad . \tag{3}$$

Eq. (2) has a simple Monte Carlo interpretation [3]. Here, we note that this equation can be viewed as an infinite-medium transport problem for each spatial cell, with cross-sections corresponding to the leakage to the cell left or right of the current cell. We define the left leakage cross-section as

$$\Sigma_{L,i} = \frac{A_{i-1/2}}{\Delta x_i} \quad , \tag{4}$$

and the right-leakage cross-section as

$$\Sigma_{R,i} = \frac{A_{i+1/2}}{\Delta x_i} \quad . \tag{5}$$

The right side of Eq. (2) contains not only the usual source term, but also source terms corresponding to particles leaking from adjacent cells into the current cell.

We now describe the previously developed Marshak interface method [1,2]. Implementing this method corresponds to developing a cell-centered equation for cell 1 (cell I can be treated in a similar manner).

The Marshak boundary condition at X_L is [4]

$$\int_0^1 \mu\psi_b(\mu)d\mu = \frac{\phi(X_L)}{4} - \frac{\lambda}{4\Sigma_t}\frac{d\phi}{dx}\bigg|_{x=X_L} \quad . \tag{6}$$

In Eq. (6) ψ_b is the angular flux incident on the interface surface (determined by the standard Monte Carlo simulation). The left side of Eq. (6) represents the partial current incident on the transport-diffusion interface, and only produces correct results in ψ_b is isotropic. In addition, λ is the *extrapolation distance*, equal to $2/3$ in the standard Marshak boundary condition. However, a more accurate value is 0.7104 [5], which we will use for the remainder of this summary.

Using Eq. (6) in a finite-difference approximation similar to the one used to develop Eq. (2), the cell-centered equation for cell 1 is [6]

$$\left(\frac{A_{3/2}}{\Delta x_1}+\frac{1}{\Delta x_1}\frac{2}{3\Sigma_{t,1}\Delta x_1+6\lambda}+\Sigma_{a,1}\right)\phi_1 = Q_1+\frac{A_{3/2}}{\Delta x_1}\phi_2 + \frac{1}{\Delta x_1}\frac{8}{3\Sigma_{t,1}\Delta x_1+6\lambda}\int_0^1 \mu\psi_b(\mu)d\mu \quad . \quad (7)$$

Eq. (7) has a Monte Carlo interpretation similar to that of Eq. (2). We denote the left-leakage cross-section (corresponding to DDMC particles leaking from cell 1 and being converted into Monte Carlo particles) as

$$\Sigma_{L,1}=\frac{2}{3\Sigma_{t,1}\Delta x_1+6\lambda} \quad . \quad (8)$$

In addition, the last term on the right side of Eq. (7) is a source term corresponding to Monte Carlo particles incident on the interface surface being converted to DDMC particles. From this term, we define the probability P of a Monte Carlo particle incident on the DDMC region being converted to a DDMC particle as

$$P=\frac{8}{3\Sigma_{t,1}\Delta x_1+6\lambda} \quad . \quad (9)$$

DDMC particles that are converted to Monte Carlo particles through "left-leakage" reactions, or Monte Carlo particles incident on the interface surface and not converted to DDMC particles, are placed on the interface surface with an outgoing isotropic angular distribution. Although this angular distribution is not correct it can be shown to be a good approximation [7].

We now present our new interface method based on the asymptotic diffusion-limit boundary condition [5]:

$$2\int_0^1 W(\mu)\psi_b(\mu)d\mu = \phi(X_L)-\frac{\lambda}{\Sigma_t}\frac{d\phi}{dx}\bigg|_{x=X_L} \quad . \quad (10)$$

Eq. (10) can be developed in an asymptotic analysis of the underlying transport equation as the mean-free path $1/\Sigma_t$ becomes small and the scattering ratio $1-\Sigma_a/\Sigma_t$ approaches unity [5]. In Eq. (10), $W(\mu)$ is a transcendental function well approximated by

$$W(\mu)\approx \mu+\frac{3}{2}\mu^2 \quad . \quad (11)$$

Using Eq. (10) in a finite-difference approximation similar to the one used to develop Eq. (7), the cell-centered equation for cell 1 is

$$\left(\frac{A_{3/2}}{\Delta x_1}+\frac{1}{\Delta x_1}\frac{2}{3\Sigma_{t,1}\Delta x_1+6\lambda}+\Sigma_{a,1}\right)\phi_1 = Q_1+\frac{A_{3/2}}{\Delta x_1}\phi_2 + \frac{1}{\Delta x_1}\frac{4}{3\Sigma_{t,1}\Delta x_1+6\lambda}\int_0^1 W(\mu)\psi_b(\mu)d\mu \quad . \quad (12)$$

Eq. (12) has a Monte Carlo interpretation similar to that of both Eqs. (2) and (7). We see that the left-leakage cross-section for cell 1 using the asymptotic boundary condition is identical to the cross-section developed from the Marshak boundary condition. However, the source term due to Monte Carlo particles incident on the interface surface is different for this new interface technique. To give this source term a Monte Carlo interpretation, we note that the rate at which Monte Carlo particles are incident on the surface for a given direction μ is $\mu\psi_b(\mu)$. Then, using the last term in Eq. (12), the angle-dependent probability that an incident Monte Carlo particle is converted to a DDMC particle is

$$P(\mu)=\frac{4}{3\Sigma_{t,1}\Delta x_1+6\lambda}\left(1+\frac{3}{2}\mu\right) \quad . \quad (13)$$

As with the Marshak interface method, the direction of particles entering the transport region is sampled isotropically.

NUMERICAL RESULTS

We now present numerical results demonstrating the increased accuracy of our new interface method based on the asymptotic boundary condition over the previously developed Marshak interface technique. In these simulations our DDMC method will consist of Eq. (2), and Eqs. (7) and (9) for the Marshak interface method, or Eqs. (12) and (13) for the new asymptotic interface method.

Our test problem is a two region slab problem suggested by Gesh and Adams [7]. This problem consists of a purely absorbing region (0 cm $< x <$ 1 cm) 1 mean-free path thick adjacent to a purely scattering region (1 cm $< x <$ 2 cm) 1000 mean-free paths thick. The right boundary of this problem has a vacuum boundary condition, while the left boundary has a normally incident angular flux.

This problem was simulated with Monte Carlo in the first region, and either Monte Carlo (which

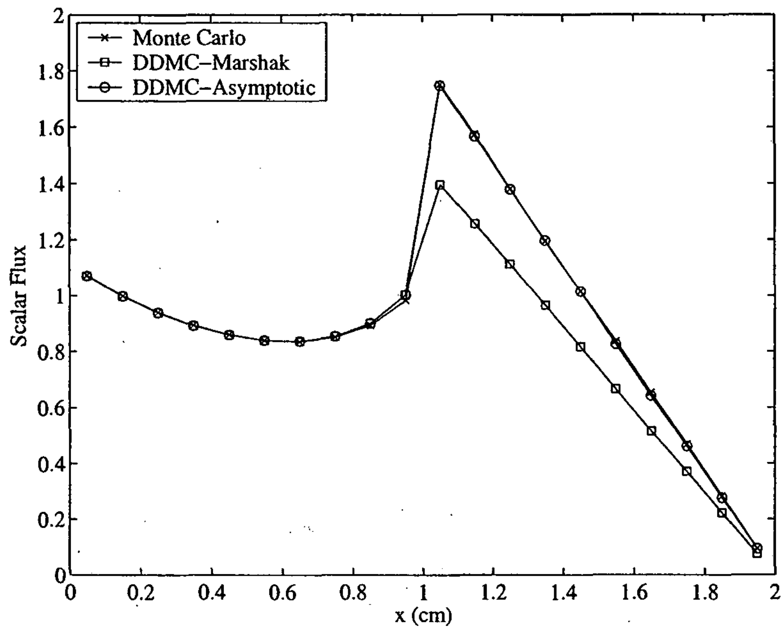

Figure 1: Interface Problem Results

provides a benchmark solution), DDMC with the Marshak interface method, or DDMC with the asymptotic interface method in the second region. A spatial mesh of Δx =0.1 cm and 10 million particles were used in each simulation.

The results of these simulations are plotted in Figure 1. From this figure we see that the asymptotic interface results agree quite well with the Monte Carlo solution, while the Marshak interface results are substantially in error, especially in the second, diffusive region. Since the angular flux on the left boundary is normally directed, and the first region is purely absorbing, the angular flux incident on the interface between the regions is also normally directed. Since the Marshak boundary condition is unable to treat this angular distribution, the results produced by the Marshak interface method will be incorrect. For this problem both DDMC simulations were nearly 100 times faster than Monte Carlo.

CONCLUSIONS

We have presented a new technique for treating the interface between standard Monte Carlo and Discrete Diffusion Monte Carlo simulations. This new technique, based on the asymptotic diffusion-limit boundary condition, is able to produce accurate results for anisotropic incident angular fluxes, a situation where the previously developed interface method based on the Marshak boundary condition is inaccurate. With a set of numerical simulations, we demonstrated this improved accuracy of our new asymptotic interface method over the Marshak interface method.

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